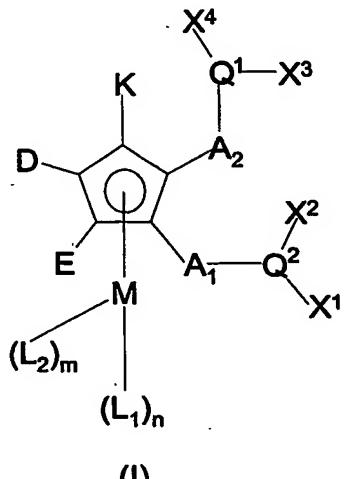


**Claims**

1. A compound obtainable by combining:

- (a) a Group VIIIB metal or a compound thereof; and,
- 5 (b) a compound of formula I or salt thereof:



wherein:

10  $A_1$  and  $A_2$ , and  $A_3$ ,  $A_4$  and  $A_5$  (when present), each independently represent lower alkylene;

$K$  is selected from the group consisting of hydrogen, lower alkyl, aryl, Het, halo, cyano, nitro,  $-OR^{19}$ ,  $-OC(O)R^{20}$ ,  
15  $-C(O)R^{21}$ ,  $-C(O)OR^{22}$ ,  $-N(R^{23})R^{24}$ ,  $-C(O)N(R^{25})R^{26}$ ,  $-C(S)(R^{27})R^{28}$ ,  
 $-SR^{29}$ ,  $-C(O)SR^{30}$ ,  $-CF_3$  or  $-A_3-Q^3(X^5)X^6$ ;

$D$  is selected from the group consisting of hydrogen, lower alkyl, aryl, Het, halo, cyano, nitro,  $-OR^{19}$ ,  $-OC(O)R^{20}$ ,  
20  $-C(O)R^{21}$ ,  $-C(O)OR^{22}$ ,  $-N(R^{23})R^{24}$ ,  $-C(O)N(R^{25})R^{26}$ ,  $-C(S)(R^{27})R^{28}$ ,  
 $-SR^{29}$ ,  $-C(O)SR^{30}$ ,  $-CF_3$  or  $-A_4-Q^4(X^7)X^8$ ;

$E$  is selected from the group consisting of hydrogen, lower alkyl, aryl, Het, halo, cyano, nitro,  $-OR^{19}$ ,  $-OC(O)R^{20}$ ,

-C(O)R<sup>21</sup>, -C(O)OR<sup>22</sup>, -N(R<sup>23</sup>)R<sup>24</sup>, -C(O)N(R<sup>25</sup>)R<sup>26</sup>, -C(S)(R<sup>27</sup>)R<sup>28</sup>,  
-SR<sup>29</sup>, -C(O)SR<sup>30</sup>, -CF<sub>3</sub> or -A<sub>5</sub>-Q<sup>5</sup>(X<sup>9</sup>)X<sup>10</sup>;

or both D and E together with the carbon atoms of the  
5 cyclopentadienyl ring to which they are attached form an  
optionally substituted phenyl ring:

X<sup>1</sup> represents CR<sup>1</sup>(R<sup>2</sup>)(R<sup>3</sup>), congressyl or adamantyl, X<sup>2</sup>  
represents CR<sup>4</sup>(R<sup>5</sup>)(R<sup>6</sup>), congressyl or adamantyl, or X<sup>1</sup> and  
10 X<sup>2</sup> together with Q<sup>2</sup> to which they are attached form an  
optionally substituted 2-phospha-adamantyl group, or X<sup>1</sup>  
and X<sup>2</sup> together with Q<sup>2</sup> to which they are attached form a  
ring system of formula 1a;

15 X<sup>3</sup> represents CR<sup>7</sup>(R<sup>8</sup>)(R<sup>9</sup>), congressyl or adamantyl, X<sup>4</sup>  
represents CR<sup>10</sup>(R<sup>11</sup>)(R<sup>12</sup>), congressyl or adamantyl, or X<sup>3</sup>  
and X<sup>4</sup> together with Q<sup>1</sup> to which they are attached form an  
optionally substituted 2-phospha-adamantyl group, or X<sup>3</sup>  
and X<sup>4</sup> together with Q<sup>1</sup> to which they are attached form a  
20 ring system of formula 1b;

X<sup>5</sup> represents CR<sup>13</sup>(R<sup>14</sup>)(R<sup>15</sup>), congressyl or adamantyl, X<sup>6</sup>  
represents CR<sup>16</sup>(R<sup>17</sup>)(R<sup>18</sup>), congressyl or adamantyl, or X<sup>5</sup>  
and X<sup>6</sup> together with Q<sup>3</sup> to which they are attached form an  
25 optionally substituted 2-phospha-adamantyl group, or X<sup>5</sup>  
and X<sup>6</sup> together with Q<sup>3</sup> to which they are attached form a  
ring system of formula 1c;

X<sup>7</sup> represents CR<sup>31</sup>(R<sup>32</sup>)(R<sup>33</sup>), congressyl or adamantyl, X<sup>8</sup>  
30 represents CR<sup>34</sup>(R<sup>35</sup>)(R<sup>36</sup>), congressyl or adamantyl, or X<sup>7</sup>  
and X<sup>8</sup> together with Q<sup>4</sup> to which they are attached form an  
optionally substituted 2-phospha-adamantyl group, or X<sup>7</sup>

and  $X^8$  together with  $Q^4$  to which they are attached form a ring system of formula 1d;

5        $X^9$  represents  $CR^{37}(R^{38})(R^{39})$ , congressyl or adamantyl,  $X^{10}$  represents  $CR^{40}(R^{41})(R^{42})$ , congressyl or adamantyl, or  $X^9$  and  $X^{10}$  together with  $Q^5$  to which they are attached form an optionally substituted 2-phospha-adamantyl group, or  $X^9$  and  $X^{10}$  together with  $Q^5$  to which they are attached form a ring system of formula 1e;

10

$Q^1$  and  $Q^2$ , and  $Q^3$ ,  $Q^4$  and  $Q^5$  (when present), each independently represent phosphorus, arsenic or antimony;

15       M represents a Group VIB or VIIIB metal or metal cation thereof;

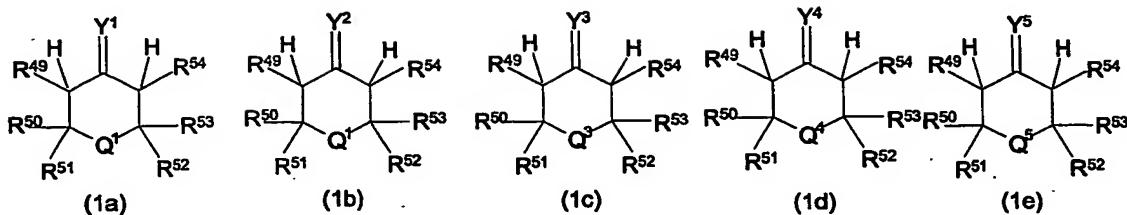
$L_1$  represents an optionally substituted cyclopentadienyl, indenyl or aryl group;

20        $L_2$  represents one or more ligands each of which are independently selected from hydrogen, lower alkyl, alkylaryl, halo, CO,  $P(R^{43})(R^{44})R^{45}$  or  $N(R^{46})(R^{47})R^{48}$ ;

25        $R^1$  to  $R^{18}$  and  $R^{31}$  to  $R^{42}$ , when present, each independently represent hydrogen, lower alkyl, aryl, halo or Het;

$R^{19}$  to  $R^{30}$  and  $R^{43}$  to  $R^{48}$ , when present, each independently represent hydrogen, lower alkyl, aryl or Het;

30       the ring systems of formula 1a, 1b, 1c, 1d and 1e are represented by the formulae



R<sup>49</sup>, R<sup>54</sup> and R<sup>55</sup>, each independently represent hydrogen, lower alkyl or aryl; R<sup>50</sup> to R<sup>53</sup> each independently represent hydrogen, lower alkyl, aryl or Het; and Y<sup>1</sup>, Y<sup>2</sup>, 5 Y<sup>3</sup>, Y<sup>4</sup> and Y<sup>5</sup>, each independently represent oxygen, sulfur or N-R<sup>55</sup>;

n = 0 or 1;

10 and m = 0 to 5;

provided that when n = 1 then m equals 0, and when n equals 0 then m does not equal 0.

15 2. A compound as claimed in claim 1, wherein if both K represents -A<sub>3</sub>-Q<sup>3</sup>(X<sup>5</sup>)X<sup>6</sup> and E represents -A<sub>5</sub>-Q<sup>5</sup>(X<sup>9</sup>)X<sup>10</sup>, then D represents -A<sub>4</sub>-Q<sup>4</sup>(X<sup>7</sup>)X<sup>8</sup>.

20 3. A compound as claimed in claim 1 or 2, wherein R<sup>1</sup> to R<sup>18</sup> and R<sup>31</sup> to R<sup>42</sup> each independently represent hydrogen, optionally substituted C<sub>1</sub>-C<sub>6</sub> alkyl or optionally substituted phenyl.

25 4. A compound as claimed in any one of claims 1 to 3, wherein R<sup>1</sup> to R<sup>18</sup> and R<sup>31</sup> to R<sup>42</sup> each independently represent hydrogen or non-substituted C<sub>1</sub>-C<sub>6</sub> alkyl.

5. A compound as claimed in any one of claims 1 to 3, wherein one or more of the groups R<sup>1</sup> to R<sup>3</sup>, R<sup>4</sup> to R<sup>6</sup>, R<sup>7</sup> to

$R^9$ ,  $R^{10}$  to  $R^{12}$ ,  $R^{13}$  to  $R^{15}$ ,  $R^{16}$  to  $R^{18}$ ,  $R^{31}$  to  $R^{33}$ ,  $R^{34}$  to  $R^{36}$ ,  $R^{37}$  to  $R^{39}$ ,  $R^{40}$  to  $R^{42}$  together with the carbon atom to which they are attached each independently form a cyclic alkyl structure.

5

6. A compound as claimed in any one of claims 1 to 3, wherein one or more of the groups  $R^1$  and  $R^2$ ,  $R^4$  and  $R^5$ ,  $R^7$  and  $R^8$ ,  $R^{10}$  and  $R^{11}$ ,  $R^{13}$  and  $R^{14}$ ,  $R^{16}$  and  $R^{17}$ ,  $R^{31}$  and  $R^{32}$ ,  $R^{34}$  and  $R^{35}$ ,  $R^{37}$  and  $R^{38}$ ,  $R^{40}$  and  $R^{41}$  together with the carbon 10 atom to which they are attached each independently form a cyclic alkyl structure.

7. A compound as claimed in any one of the preceding claims, wherein each of  $R^1$  to  $R^{18}$  and  $R^{31}$  to  $R^{42}$  does not 15 represent hydrogen.

8. A compound as claimed in any one of the preceding claims, wherein adamantyl represents unsubstituted adamantyl or adamantyl substituted with one or more 20 unsubstituted  $C_1-C_8$  alkyl substituents, or a combination thereof.

9. A compound as claimed in any one of the preceding claims, wherein 2-phospha-adamantyl represents 25 unsubstituted 2-phospha-adamantyl or 2-phospha-adamantyl substituted with one or more unsubstituted  $C_1-C_8$  alkyl substituents, or a combination thereof.

10. A compound as claimed in any one of the preceding 30 claims, wherein 2-phospha-adamantyl includes one or more oxygen atoms in the 2-phospha-adamantyl skeleton.

11. A compound as claimed in any one of the preceding claims, wherein congressyl represents unsubstituted congressyl.

5 12. A compound as claimed in any one of the preceding claims, wherein R<sup>50</sup> to R<sup>53</sup> each independently represent optionally substituted C<sub>1</sub>-C<sub>6</sub> alkyl, trifluoromethyl or phenyl optionally substituted with non-substituted C<sub>1</sub>-C<sub>6</sub> alkyl or OR<sup>19</sup> where R<sup>19</sup> represents non-substituted C<sub>1</sub>-C<sub>6</sub> alkyl.

10 13. A compound as claimed in any one of the preceding claims, wherein R<sup>49</sup> and R<sup>54</sup> each independently represent hydrogen or non-substituted C<sub>1</sub>-C<sub>6</sub> alkyl.

15 14. A compound as claimed in any one of the preceding claims, wherein each of Y<sup>1</sup> to Y<sup>5</sup> represents oxygen.

20 15. A compound as claimed in any one of the preceding claims, wherein X<sup>1</sup> is identical to X<sup>3</sup>, and X<sup>5</sup>, X<sup>7</sup> and X<sup>9</sup> when present.

25 16. A compound as claimed in any one of the preceding claims, wherein X<sup>2</sup> is identical to X<sup>4</sup>, and X<sup>6</sup>, X<sup>8</sup> and X<sup>10</sup> when present.

17. A compound as claimed in any one of claims 1 to 14, wherein X<sup>1</sup> represents CR<sup>1</sup>(R<sup>2</sup>)(R<sup>3</sup>), X<sup>2</sup> represents CR<sup>4</sup>(R<sup>5</sup>)(R<sup>6</sup>), X<sup>3</sup> represents CR<sup>7</sup>(R<sup>8</sup>)(R<sup>9</sup>) and X<sup>4</sup> represents CR<sup>10</sup>(R<sup>11</sup>)(R<sup>12</sup>).

18. A compound as claimed in any one of claims 1 to 14, wherein  $X^1$  represents  $CR^1(R^2)(R^3)$ ,  $X^2$  represents adamantyl,  $X^3$  represents  $CR^7(R^8)(R^9)$  and  $X^4$  represents adamantyl.

5 19. A compound as claimed in any one of claims 1 to 14, wherein  $X^1$  represents  $CR^1(R^2)(R^3)$ ,  $X^2$  represents congressyl,  $X^3$  represents  $CR^7(R^8)(R^9)$  and  $X^4$  represents congressyl.

10 20. A compound as claimed in any one of claims 1 to 14, wherein  $X^1$  to  $X^4$  each independently represent adamantyl.

21. A compound as claimed in any one of claims 1 to 14, wherein  $X^1$  to  $X^4$  each independently represent congressyl.

15

22. A compound as claimed in any one of claims 1 to 14, wherein  $X^1$  and  $X^2$  together with  $Q^2$  to which they are attached form a ring system of formula Ia, and  $X^3$  and  $X^4$  together with  $Q^1$  to which they are attached form a ring system of formula Ib.

23. A compound as claimed in any one of claims 1 to 14, wherein  $X^1$  and  $X^2$  together with  $Q^2$  to which they are attached form a 2-phospha-adamantyl group, and  $X^3$  and  $X^4$  together with  $Q^1$  to which they are attached form a 2-phospha-adamantyl group.

24. A compound as claimed in any one of the preceding claims, wherein K represents hydrogen.

30

25. A compound as claimed in any one of claims 1 to 23, wherein K represents  $-A_3-Q^3(X^5)X^6$ .

26. A compound as claimed in claim 25, wherein  $-A_3-Q^3(X^5)X^6$  is identical to  $-A_2-Q^1(X^3)X^4$ .

27. A compound as claimed in any one of the preceding  
5 claims, wherein D and E together with the carbon atoms of  
the cyclopentadienyl ring to which they are attached form  
an unsubstituted phenyl ring.

28. A compound as claimed in any one of the preceding  
10 claims, wherein D and E both represent hydrogen.

29. A compound as claimed in any one of claims 1 to 26,  
wherein D represents  $-A_4-Q^4(X^7)X^8$ .

15 30. A compound as claimed in claim 29, wherein  $-A_4-Q^4(X^7)X^8$  is identical to  $-A_2-Q^1(X^3)X^4$ .

31. A compound as claimed in any one claims 29 or 30,  
wherein E represents hydrogen.

20

32. A compound as claimed in any one claims 1 to 26, 29  
or 30, wherein E represents  $-A_5-Q^5(X^9)X^{10}$ .

25 33. A compound as claimed in claim 32, wherein  $-A_5-Q^5(X^9)X^{10}$  is identical to  $-A_2-Q^1(X^3)X^4$ .

34. A compound as claimed in any one of the preceding  
claims, wherein  $A_1$  and  $A_2$ , and  $A_3$ ,  $A_4$  and  $A_5$  when present,  
each independently represent  $-CH_2-$  or  $-C_2H_4-$ .

30

35. A compound as claimed in any one of the preceding  
claims, wherein each  $A_1$  and  $A_2$ , and  $A_3$ ,  $A_4$  and  $A_5$  when  
present are identical and preferably represent  $-CH_2-$ .

36. A compound as claimed in any one of the preceding claims, wherein each Q<sup>1</sup> and Q<sup>2</sup>, and Q<sup>3</sup>, Q<sup>4</sup> and Q<sup>5</sup> when present are identical and preferably represent phosphorous.

37. A compound as claimed in any one of the preceding claims, wherein n=1, m=0 and L<sub>1</sub> is selected from cyclopentadienyl, phenyl, indenyl or napthyl, preferably unsubstituted cyclopentadienyl.

38. A compound as claimed in any one of the preceding claims, wherein M represents iron or a metal cation thereof.

15

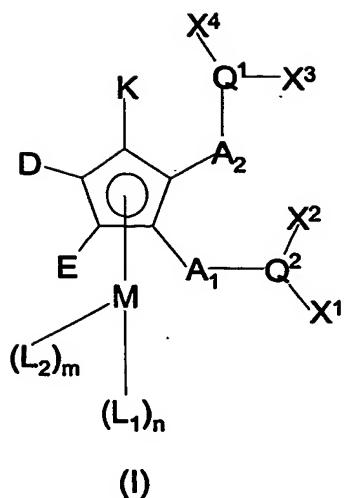
39. A compound as claimed in any one of the preceding claims obtainable by combining: (a) palladium or a compound thereof; and (b) a compound of formula I as defined in any one of the preceding claims.

20

40. A process for preparing a compound as defined in any one of claims 1 to 39 comprising combining (a) a Group VIIIB metal or compound thereof; and, (b) a compound of formula I as defined in any one of claims 1 to 38.

25

41. A compound of formula I



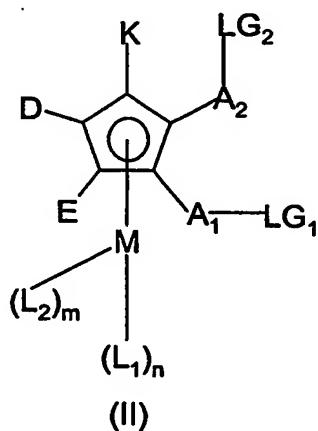
(I)

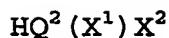
wherein A<sub>1</sub>, A<sub>2</sub>, K, D, E, M, L<sub>2</sub>, L<sub>1</sub>, Q<sup>1</sup>, Q<sup>2</sup>, X<sup>1</sup>, X<sup>2</sup>, X<sup>3</sup>, X<sup>4</sup>, n and m are as defined in any one of claims 1 to 38.

5

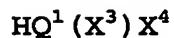
42. A process for preparing a compound of formula I as defined in claim 41, comprising reacting a compound of formula II wherein A<sub>1</sub>, A<sub>2</sub>, K, D, E, M, L<sub>1</sub>, L<sub>2</sub>, n and m are as defined for a compound of formula I, and LG<sub>1</sub> and LG<sub>2</sub> represent suitable leaving groups, with a compound of formula IIIa and IIIb

10





(IIIa)

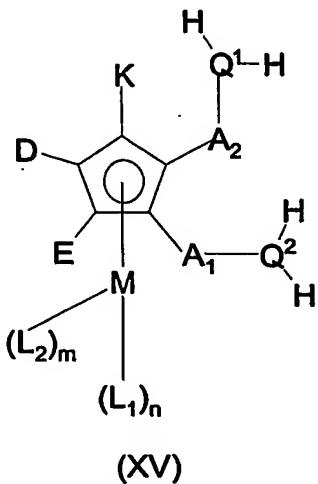


(IIIb)

5 wherein  $\text{X}^1$ ,  $\text{X}^2$ ,  $\text{Q}^2$ ,  $\text{X}^3$ ,  $\text{X}^4$  and  $\text{Q}^1$  are as defined in anyone  
of claims 1 to 38.

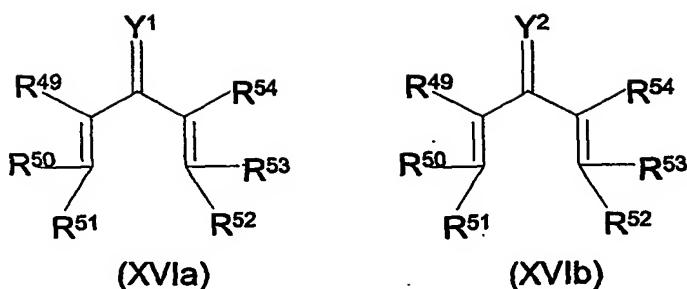
43. A compound of formula II as defined in claim 42.

10 44. A process for preparing a compound of formula I  
wherein K, D, E, M,  $\text{A}_2$ ,  $\text{A}_1$ ,  $\text{L}_2$ ,  $\text{L}_1$ ,  $\text{Q}^1$ ,  $\text{Q}^2$ , m and n are as  
defined in any one of claims 1 to 38 and  $\text{X}^1$  and  $\text{X}^2$   
together with  $\text{Q}^2$  to which they are attached form a ring  
system of formula Ia as defined in anyone of claims 1 to  
15 38 and  $\text{X}^3$  and  $\text{X}^4$  together with  $\text{Q}^1$  to which they are  
attached form a ring system of formula Ib as defined in  
any one of claims 1 to 38, comprising reacting a compound  
of formula XV



20

wherein K, D, E, M,  $\text{A}_2$ ,  $\text{A}_1$ ,  $\text{L}_2$ ,  $\text{L}_1$ ,  $\text{Q}^1$ ,  $\text{Q}^2$ , m and n are as  
defined in any one of claims 1 to 38, with a compound of  
formula XVIa and XVIb



wherein Y<sup>1</sup>, Y<sup>2</sup>, R<sup>49</sup> to R<sup>55</sup> are as defined for a compound of formula I.

5

45. A compound of formula XV as defined in claim 44.

46. A process for the carbonylation of an ethylenically unsaturated compound comprising contacting an ethylenically unsaturated compound with carbon monoxide and a co-reactant in the presence of a compound as defined in any one of claims 1 to 39.

47. A process as defined in claim 46 wherein the co-  
15 reactant includes a hydroxyl group containing compound.

48. A process as claimed in claim 46 or 47 wherein the ethylenically unsaturated compound comprises ethylene, 1,3-butadiene, oct-1-ene or vinyl acetate, preferably  
20 ethylene.

49. A process as claimed in any one of claims 46 to 48, further including the step of including a source of anions.

25

50. A composition comprising a compound as defined in any one of claims 1 to 39 attached to a support.

51. Use of a compound as defined in anyone of claims 1 to 39 or a composition as defined in claim 50 as a catalyst.